How to Understand and Tune HPC I/O Performance

ATPESC 2021

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Surveying the HPC I/O landscape

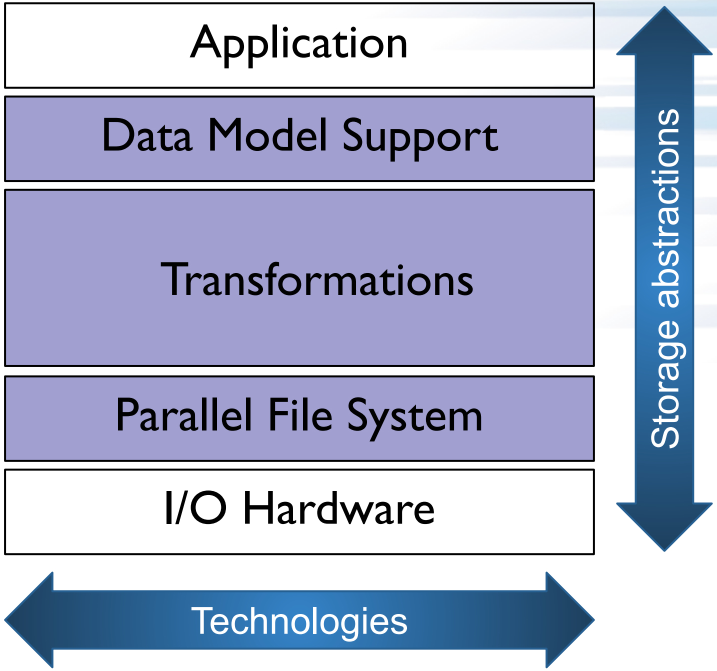
A complex data management ecosystem

As evidenced by today's presentations, the HPC I/O landscape is deep and vast

- High-level data abstractions: HDF5, PnetCDF
- Parallel file systems: Lustre, GPFS
- Storage hardware: HDDs, SSDs, NVM

Application developers tend to prefer high-level data models for convenience, but these APIs often obfuscate the behavior of lower level interfaces that drive I/O performance

Understanding I/O behavior in this environment is difficult, much less turning observations into actionable I/O tuning decisions

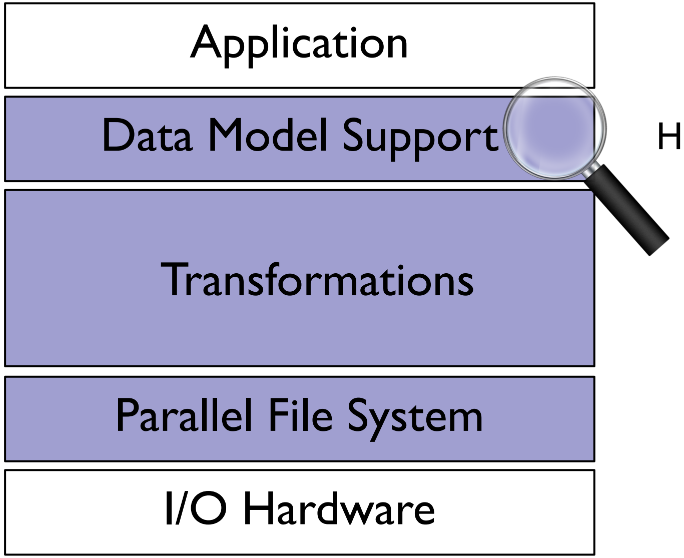


Characterizing HPC I/O workloads with Darshan

A look under the hood of an HPC application

You have already heard some basics about Darshan, a powerful tool for users to better understand and tune their I/O workloads

Darshan provides many helpful stats across multiple layers of the I/O stack that are critical to understanding application I/O behavior



HDF5 file stats*:

- Metadata operation counts (open, flush)
- MPI-IO usage
- Metadata timing

*Note: Detailed HDF5 instrumentation can be optionally enabled only for Darshan versions 3.2.0+

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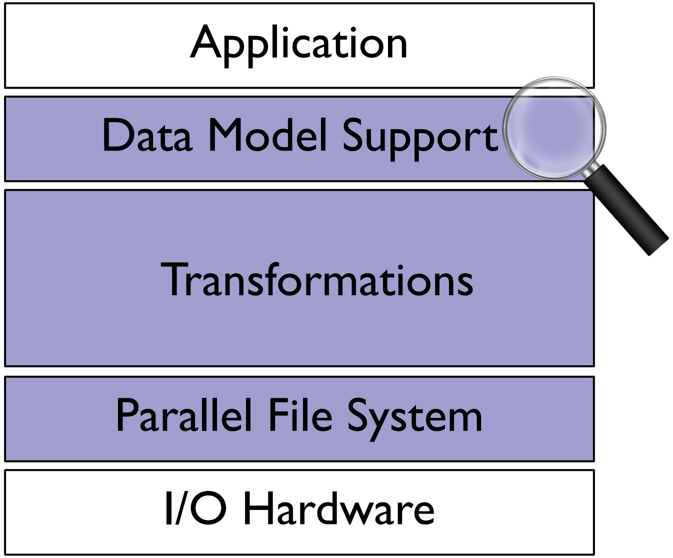

HDF5 dataset stats*:

- Data operation counts (read, write)
- Metadata operation counts (open, flush)
- Total I/O volumes (read, write)
- Common access info (size, hyperslab parameters)
- Chunking parameters
- Dataspace total dimensions, points
- MPI-IO collective usage
- Data & metadata timing

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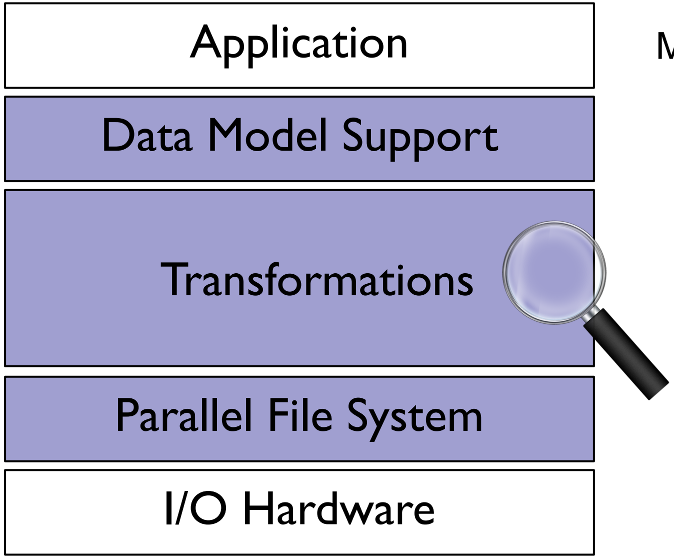

MPI-IO file stats:

- Data operation counts (read, write, sync)
- Metadata operation counts (open)
- Collective and independent
- Total I/O volumes (read, write)
- Access size info
  - Common values
  - Histograms
- Data & metadata timing

Hands on exercises: https://github.com/radix-io/hands-on

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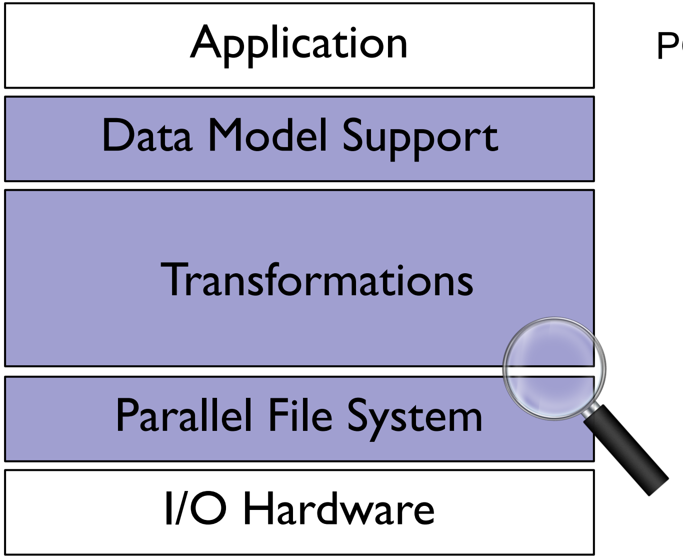

POSIX file stats:

- Data operation counts (read, write, sync)
- Metadata operation counts (open, seek, stat)
- Total I/O volumes (read, write)
- File alignment
- Access size/stride info
  - Common values
  - Histograms
- Data & metadata timing

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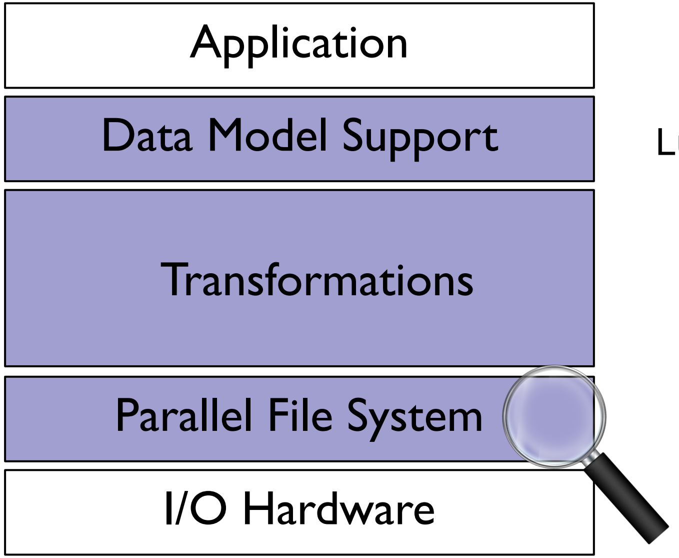

Lustre file stats:

- Data server (OST) and metadata server (MDT) counts
- Stripe size/width
- OST list serving a file

Characterizing HPC I/O workloads with Darshan

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Application
Data Model Support
Transformations
Parallel File System
I/O Hardware

Let's see how Darshan can be leveraged in some practical use cases that demonstrate some widely held best practices in tuning HPC I/O performance

Tuning the parallel file system

Ensuring storage resources match application I/O needs

For some parallel file systems like Lustre, users have direct control over file striping parameters

Bad news: Users may have to have some knowledge of the file system to get good I/O performance

Good news: Users can often get higher I/O performance than system defaults with thoughtful tuning -- file systems aren't perfect for every workload!

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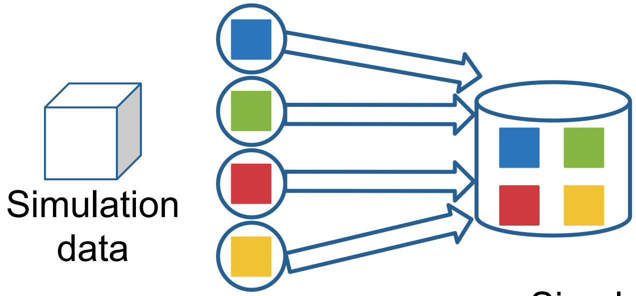

Simulation clients write data to 1 storage server

Tuning the parallel file system

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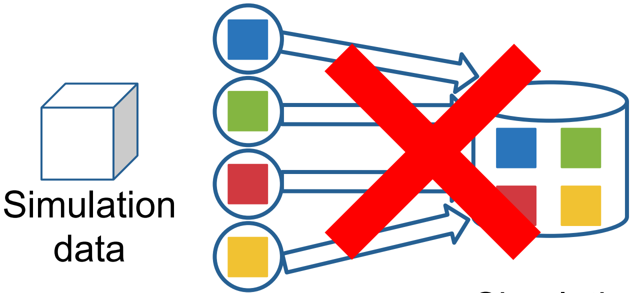
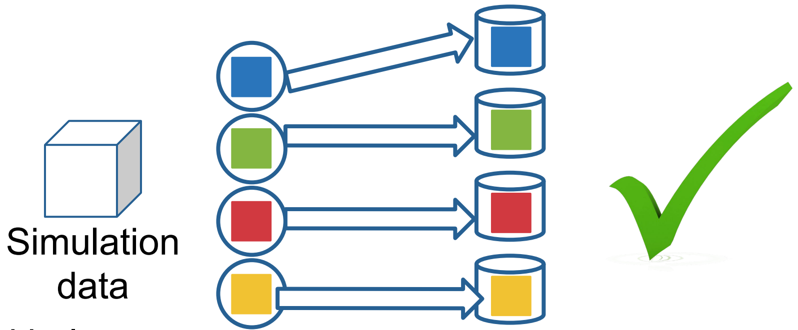




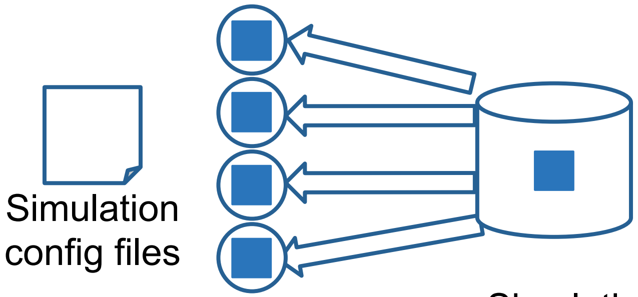
Simulation clients load balance writes across multiple servers

Tuning the parallel file system

Ensuring storage resources match application I/O needs

Tuning decisions can and should be made independently for different file types

While large application datasets should ideally be distributed across as many storage resources as possible, smaller files tend to benefit from being contained to a single server



Simulation clients read config data from 1 storage server

Tuning the parallel file system

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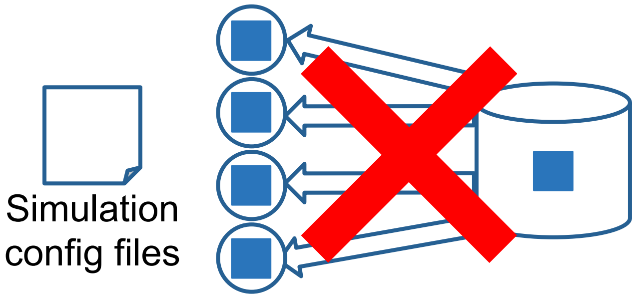

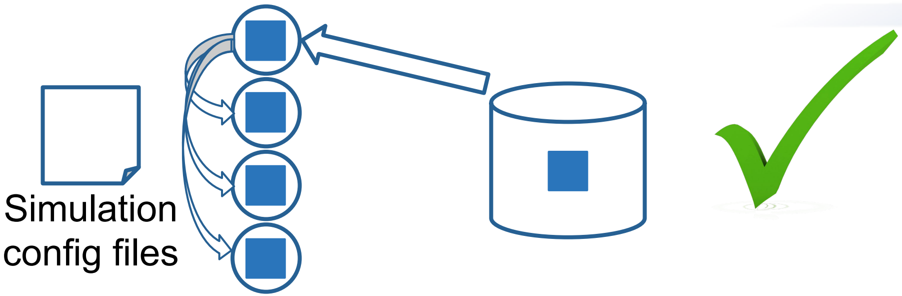

Better yet, limit storage contention by having 1 client read data and distribute using communication (e.g., MPI)

Tuning the parallel file system

Ensuring storage resources match application I/O needs

Be aware of what file system settings are available to you and don’t assume system defaults are always the best… you might be surprised what you find

- ALCF’S Theta and NERSC’s Cori default Lustre stripe width is 1

Darshan output from a simple 10-process (10-node) POSIX I/O workload to shared file on a Cori’s Lustre scratch volume:

jobid: 32840482	uid: 69628	nprocs: 10	runtime: 6 seconds

I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 210.38 MiB/s

```
LUSTRE_STRIPE_SIZE  1048576 /global/cscratc
LUSTRE_STRIPE_WIDTH 1    /global/cscratch1/s
LUSTRE_OST_ID_0 100 /global/cscratch1/sd/ss
```

Tuning the parallel file system

Ensuring storage resources match application I/O needs

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I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 210.38 MiB/s

```
> lfs setstripe -c 10 testFile # change stripe width to 10
```

jobid: 32840482	uid: 69628	nprocs: 10	runtime: 3 seconds

I/O performance *estimate* (at the POSIX layer): transferred 1000.0 MiB at 562.48 MiB/s

```
LUSTRE_STRIPE_SIZE  1048576 /global/cscrat
LUSTRE_STRIPE_WIDTH 10  /global/cscratch1/
LUSTRE_OST_ID_0 220 /global/cscratch1/sd/s
LUSTRE_OST_ID_1 146 /global/cscratch1/sd/s
LUSTRE_OST_ID_2 107 /global/cscratch1/sd/s
LUSTRE_OST_ID_3 181 /global/cscratch1/sd/s
LUSTRE_OST_ID_4 47  /global/cscratch1/sd/s
LUSTRE_OST_ID_5 209 /global/cscratch1/sd/s
LUSTRE_OST_ID_6 244 /global/cscratch1/sd/s
LUSTRE_OST_ID_7 112 /global/cscratch1/sd/s
LUSTRE_OST_ID_8 36  /global/cscratch1/sd/s
LUSTRE_OST_ID_9 154 /global/cscratch1/sd/s
```

~200% performance boost

Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Users may also need to pay close attention to file system alignment when crafting I/O accesses to a file

- Accesses that cross alignment boundaries likely perform worse than nicely aligned I/O

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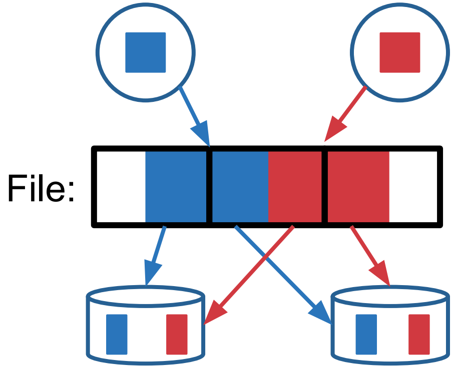
For Lustre, performance can be maximized by aligning I/O to stripe boundaries:



Unaligned I/O requests can span multiple servers and introduce inefficiencies in storage protocols

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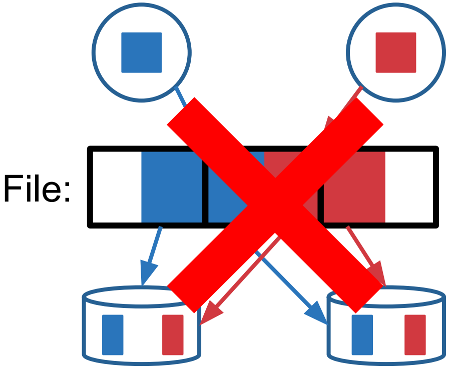
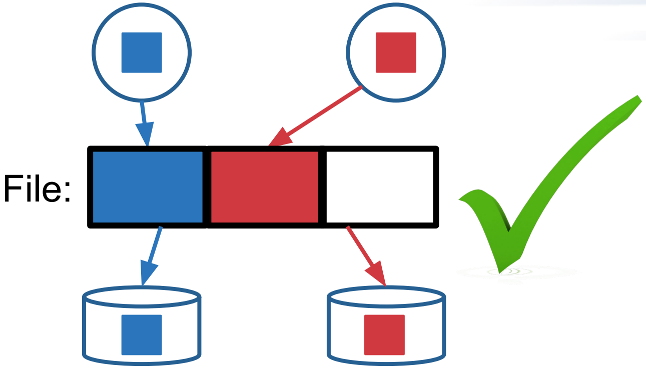


Instead, ensure client accesses are well-aligned to avoid Lustre server contention



Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Repeating our simple 10-client example striping a single file across 10 Lustre OSTs

Unaligned:

transferred 1000.0 MiB at 310.14 MiB/s

# Module	Rank	Wt/Rd	Segment	Offset	Length	Start(s)	End(s)	[OST]	
X_POSIX	0	write	0	524288	1048576	0.0065	0.0594	[32]	[197]
X_POSIX	1	write	0	1572864	1048576	0.0065	0.0538	[197]	[237]
X_POSIX	2	write	0	2621440	1048576	0.0070	0.0440	[237]	[26]
X_POSIX	3	write	0	3670016	1048576	0.0067	0.0485	[26]	[213]

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Aligned:

transferred 1000.0 MiB at 380.28 MiB/s

# Module	Rank	Wt/Rd	Segment	Offset	Length	Start(s)	End(s)	[OST]
X_POSIX	0	write	0	0	1048576	0.0054	0.0066	[197]
X_POSIX	1	write	0	1048576	1048576	0.0053	0.0064	[102]
X_POSIX	2	write	0	2097152	1048576	0.0061	0.0072	[106]
X_POSIX	3	write	0	3145728	1048576	0.0053	0.0064	[120]

Tuning low-level (POSIX) file I/O

Making efficient use of a no-frills I/O API

Even in this small workload, we pay a nearly 20% performance penalty when I/O accesses are not aligned to file stripes (1 MB)

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Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

Recall that HDF5 provides a chunking mechanism to partition user datasets into contiguous chunks in the underlying file

- Users can greatly improve performance of partial dataset I/O operations by choosing chunking parameters that match expected access patterns

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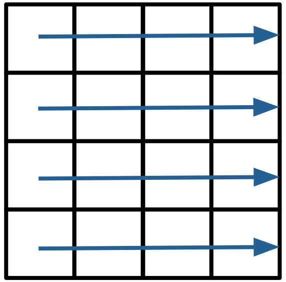

By default, HDF5 will store the dataset contiguously row-by-row (i.e., row-major format) in the file

Tuning high-level (HDF5) data access

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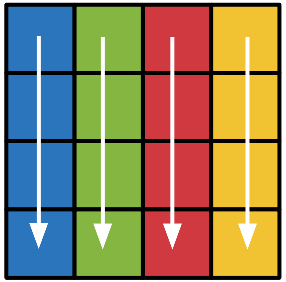
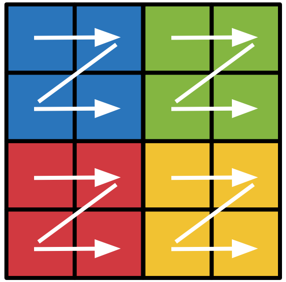


column-based



block-based

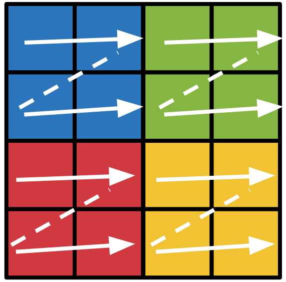
If dataset access patterns do not suit a simple row-major storage scheme, chunking can be applied to map chunks of dataset data to contiguous regions in the file

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

Consider a 256-process (16-node) example where each process exclusively accesses a block of the dataset

- Each process writes a 2048x2048 block of the dataset (32 MB per-process, 8 GB total)



With no chunking, each process issues many smaller non-contiguous I/O requests to write their block, yielding low I/O performance

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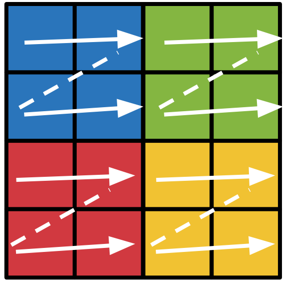
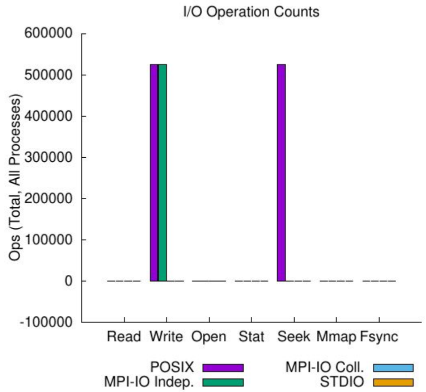


jobid: 32972116	uid: 69628	nprocs: 256	runtime: 143 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 57.97 MiB/s



Most Common Access Sizes (POSIX or MPI-IO)

	access size	count
POSIX	16384	524288
	96	2
	544	1
	328	1

256 individual HDF5 writes (1-per-process) yields 500K+ POSIX writes

Tuning high-level (HDF5) data access

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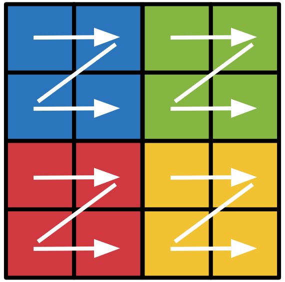

With chunking applied, each process can read their entire data block using one large, contiguous access in the file

Hands on exercises: https://github.com/radix-io/hands-on

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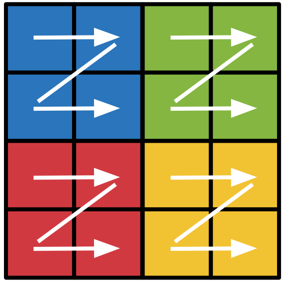
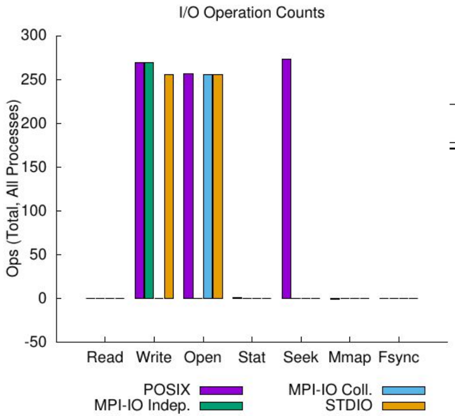


jobid: 32972116	uid: 69628	nprocs: 256	runtime: 52 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 164.73 MiB/s



Most Common Access Sizes (POSIX or MPI-IO)

	access size	count
POSIX	33554432	256
	2616	6
	96	2
	544	1

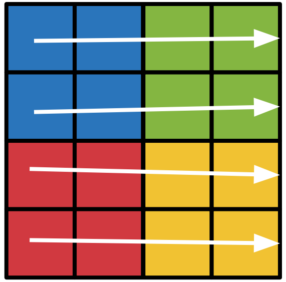
Appropriate chunking selection yields 2.8x performance increase

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

An alternative optimization relies on collective I/O to improve the efficiency of this block-style data access

- Rely on MPI-IO layer collective buffering algorithm to generate contiguous storage accesses and to limit number of clients interacting with storage system



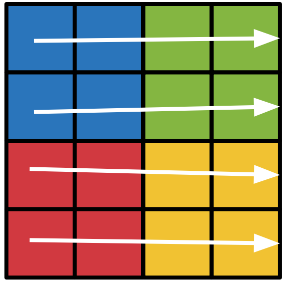
With collective I/O enabled, designated aggregator processes perform I/O on behalf of their peers, and communicate their data using MPI calls

Tuning high-level (HDF5) data access

Optimizing application interactions with the I/O stack

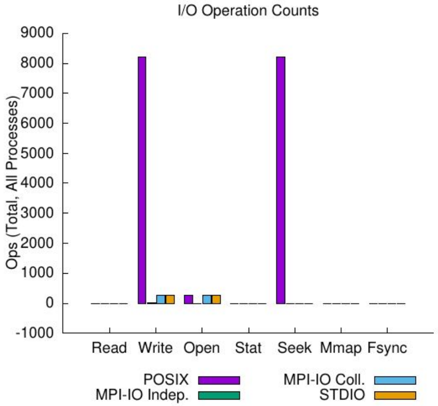
Consider a 256-process (16-node) example where each process exclusively accesses a block of the dataset

- Each process writes a 2048x2048 block of the dataset (32 MB per-process, 8 GB total)



jobid: 32972116	uid: 69628	nprocs: 256	runtime: 32 seconds

I/O performance *estimate* (at the MPI-IO layer): transferred 8192.0 MiB at 268.28 MiB/s



Most Common Access Sizes
(POSIX or MPI-IO)

	access size	count
POSIX	1048576	8191
	96	2
	1046528	1
	2048	1

Collective I/O yields 4.6x improvement over no chunking, and 1.6x improvement over chunking

Argonne NATIONAL LABORATORY
ECP EXASCALE COMPUTING PROJECT

Using Darshan to analyze HDF5 apps

Collective vs independent I/O behavior

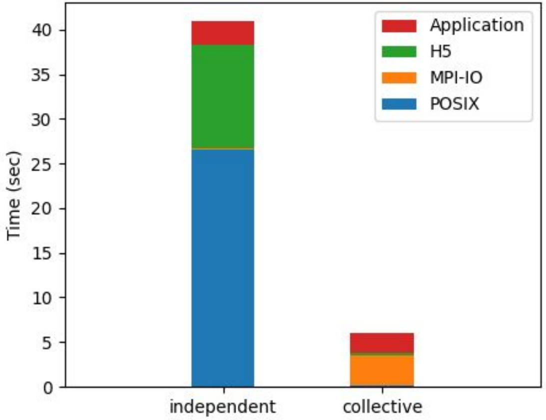
Using the MACSio[1] HDF5 benchmark, run a couple of simple examples demonstrating the types of insights HDF5 I/O instrumentation can enable

- 60-process (5-node) single shared file, 3d mesh, write roughly 1 GiB of cumulative H5D data
- Compare performance of collective and independent I/O configurations

b/w: **~30 MB/sec**

POSIX I/O dominates, **H5** incurs non-negligible overhead forming this workload

Negligible time spent in **MPI-IO**



b/w: **~290 MB/sec**

H5 and **POSIX** incur minimal overhead for this workload

MPI-IO collective I/O algorithm dominates

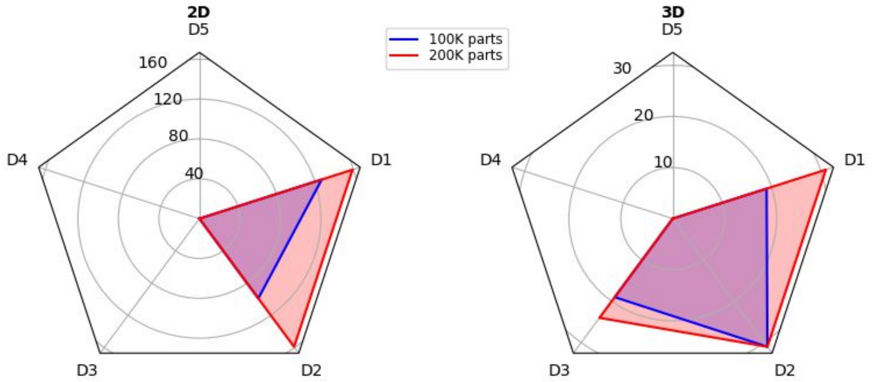
1. https://github.com/LLNL/MACSio

Using Darshan to analyze HDF5 apps

Dataset access patterns

Using the MACSio[1] HDF5 benchmark, run a couple of simple examples demonstrating the types of insights HDF5 I/O instrumentation can enable

- 60-process (5-node) single shared file, 3d mesh, write roughly 1 GiB of cumulative H5D data
- Compare dataset access patterns across different configurations



Number of elements accessed in each dataset dimension for the most common access for each MACSio configuration

Radar plots, or other methods, can be used to help visualize characteristics of HDF5 dataset accesses

Dataset access patterns could be used to help set/optimize chunking parameters to limit accesses to as few chunks as possible

1. https://github.com/LLNL/MACSio

Summarizing I/O tuning options

As a user of I/O interface X, what tuning vectors do I have?

I/O Interface	Striping	Alignment	Collective I/O	Chunking
HDF5	✓	✓	✓	✓
PnetCDF	✓	✓	✓	X
MPI-IO	✓	✓	✓	X
POSIX	✓	✓-	X	X

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POSIX	✓	✓ -	X	X

Automatically align application data and library metadata, if user requests so

Collective I/O can be automatically aligned

POSIX I/O requires manually aligning every access

Summarizing I/O tuning options

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MPI-IO	✓	✓	✓	X
POSIX	✓	✓-	X	X

In general, users should try to take advantage of high-level I/O libraries:

- I/O optimization strategies like collective I/O & chunking can net large performance gains, especially when combined with striping and alignment optimizations

Accounting for a changing HPC landscape

Adapting to technological shifts

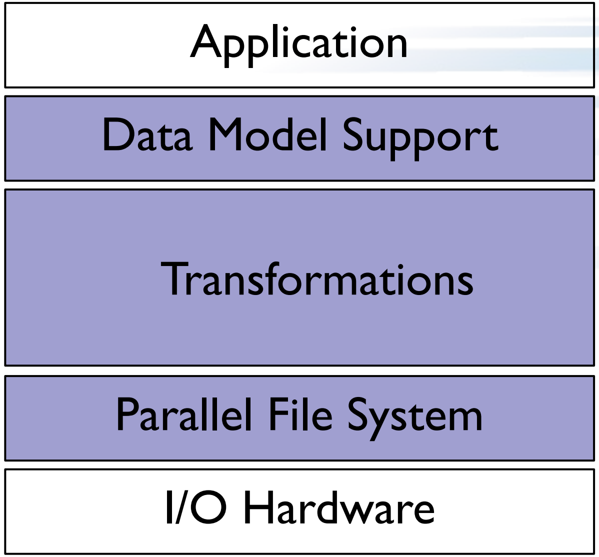
The various technologies covered today form much of the foundation of the traditional HPC data management stack

- Variations on this stack have been deployed at HPC facilities and leveraged by users for high-performance parallel I/O for decades

But, the HPC computing landscape is changing, even if slowly

Changes driven at both ends of the stack

- Newly embraced compute paradigms
- Emerging storage technologies



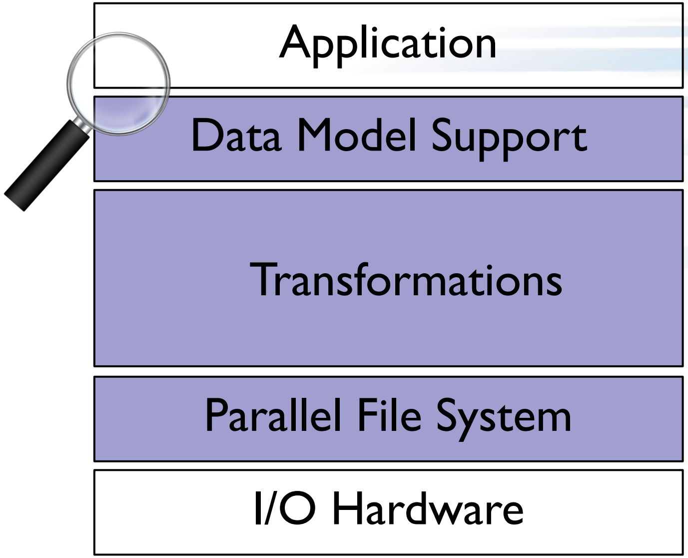
Accounting for a changing HPC landscape

Adapting to technological shifts

Large-scale MPI applications are still the norm at most most HPC centers, but other non-MPI compute frameworks are gaining traction:

- Deep learning (TensorFlow, Keras, PyTorch)
- Data analytics frameworks (Spark, Dask)
- Other non-MPI distributed computing frameworks (Legion, UPC)

Many of these frameworks define their own data models and have their own mechanisms for managing distributed tasks



Instrumenting non-MPI applications with Darshan

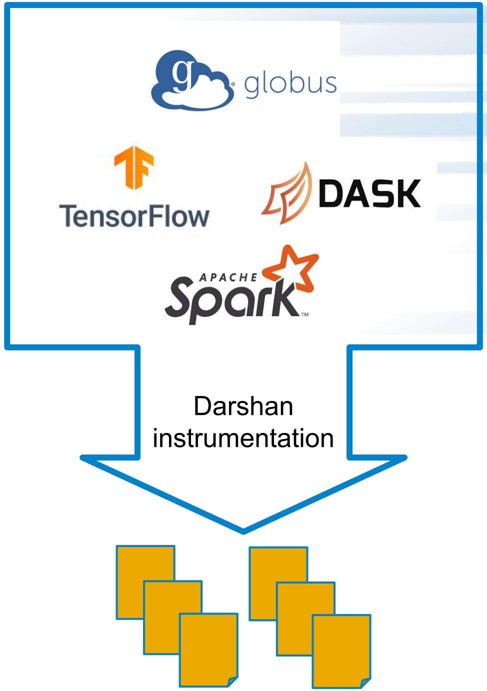
Starting with Darshan version 3.2.0, Darshan supports instrumentation of non-MPI applications*

- Just set DARSHAN_ENABLE_NONMPI environment variable before running

Generates unique Darshan log for every process invoked

Extend Darshan instrumentation from traditional MPI applications to any type of executable

- Python frameworks
- File transfer utilities
- Data service daemons
- Other serial applications



*1 caveat: applications must be dynamically-linked

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Accounting for a changing HPC landscape

Adapting to technological shifts

HPC storage technology is changing to meet needs of diverse application workloads

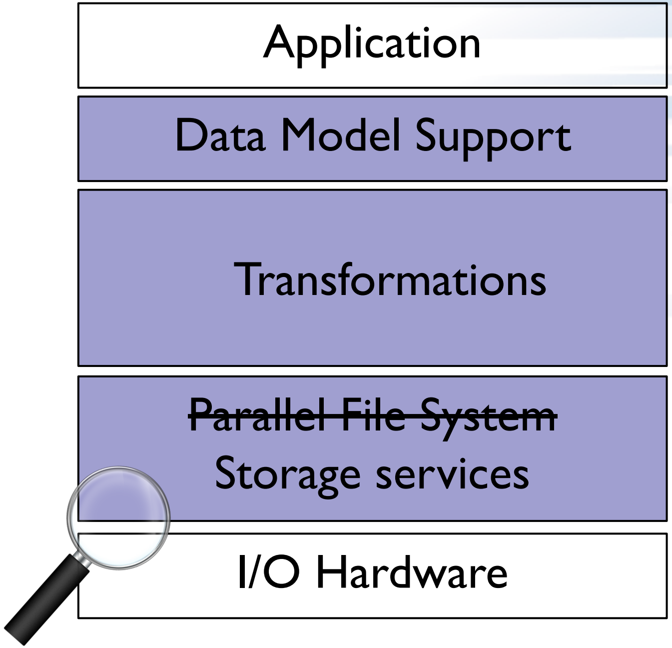
- Users typically have more options than a traditional parallel file system over HDDs

Hardware trends enabling low-latency, high-bandwidth I/O to applications

- Burst buffers, NVM

Novel storage services offer compelling alternatives to traditional file systems

- Unify, DAOS



PyDarshan: simplifying Darshan log file analysis

Darshan has traditionally offered only the C-based darshan-util library and a handful of corresponding utilities to users

- Development of custom Darshan analysis utilities is cumbersome, requiring users to either:
  - Develop analysis tools in C using the low-level darshan-util library
  - Perform an inconvenient conversion from `darshan-parser` text output

PyDarshan has been developed* to simplify the interfacing of analysis tools with Darshan log data

- Use Python CFFI module to provide Python bindings to the native darshan-utils C API
- Expose Darshan log data as dictionaries, pandas dataframes, and numpy arrays

We are hopeful PyDarshan will lead to a richer ecosystem for Darshan log analysis utilities

* Thanks to **Jakob Luettgau (DKRZ)** for contributing most of the PyDarshan code, examples, and documentation

PyDarshan: simplifying Darshan log file analysis

We've already found Jupyter notebooks to be an effective way of sharing PyDarshan analysis examples (code, documentation, visualizations) with users, collaborators, etc.

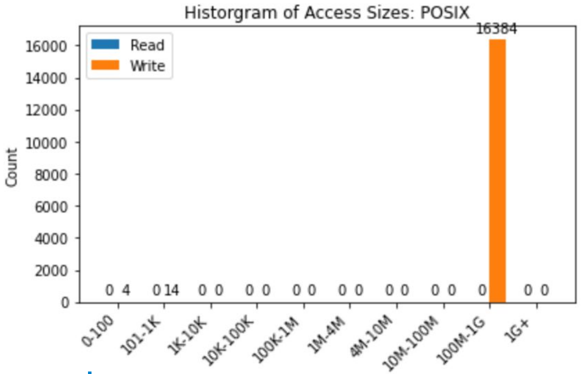
In [1]:
```
import darshan

report = darshan.DarshanReport("example-logs/example.darshan", read_all=True)  # Default
report.info()
```

```
Filename:       example-logs/example.darshan
Times:          2017-03-20 04:07:47 to 2017-03-20 04:09:43 (Duration 0:01:56)
Executeable:    /global/project/projectdirs/m888/glock/tokio-abc-results/bin.edison/vpic
rs/glock/tokioabc-s.4478544/vpicio/vpicio.hdf5 32
Processes:      2048
JobID:          4478544
UID:            69615
Modules in Log: ['POSIX', 'MPI-IO', 'LUSTRE', 'STDIO']
Loaded Records: {'POSIX': 1, 'MPI-IO': 1, 'STDIO': 1, 'LUSTRE': 1}
Name Records:   4
Darshan/Hints:  {'lib_ver': '3.1.3', 'h': 'romio_no_indep_rw=true;cb_nodes=4'}
DarshanReport:  id(140124449925824) (tmp)
```

In [3]:
```
# access histograms
plt = plot_access_histogram(report, 'POSIX')
plt.show()
```

```
Summarizing... iohist POSIX
```



Check the Darshan GitHub repo for PyDarshan examples, notebooks, etc.

https://github.com/darshan-hpc/darshan

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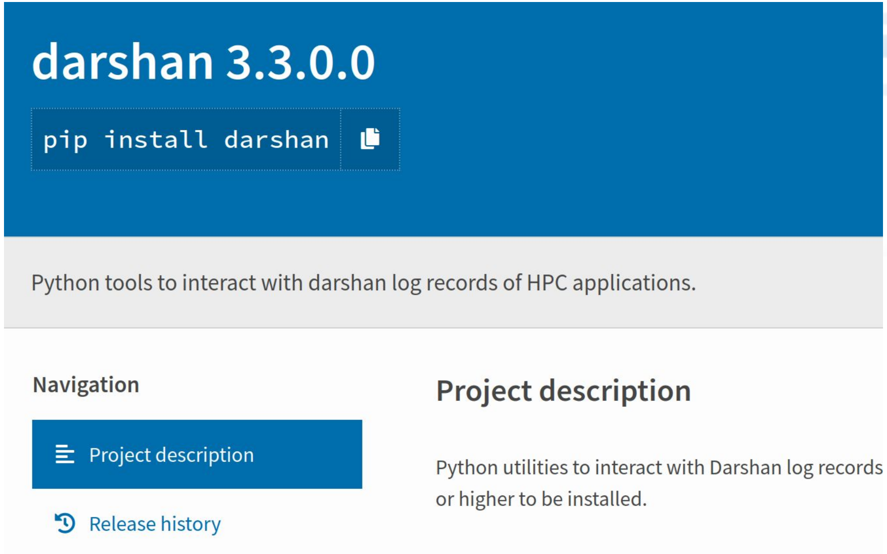
PyDarshan: simplifying Darshan log file analysis

PyDarshan is currently available on PyPI and ready for users to analyze Darshan logs with

- Use ‘`pip install darshan`’ to install the PyDarshan module from PyPI on your system
- Alternatively, PyDarshan can be installed directly from the Darshan source, by running ’`python3 setup.py install --user`‘ from the ‘darshan-util/pydarshan’ directory



Wrapping up

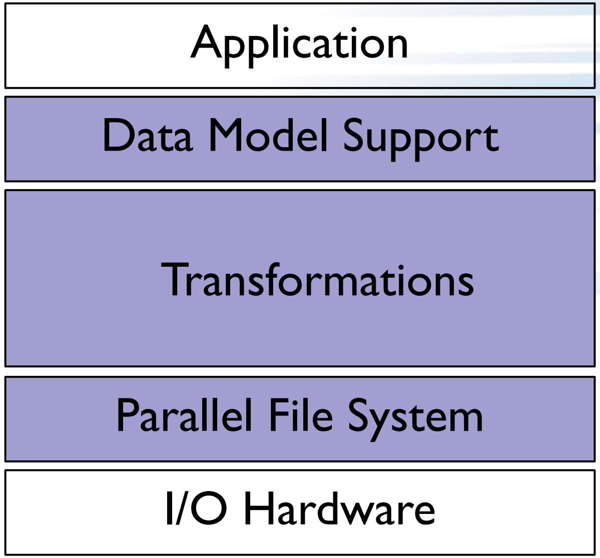
Hopefully this material proves useful in providing a deeper understanding of the different layers of the HPC I/O stack covered today, as well as potential tuning vectors available to you as user

- Optimizing your I/O workload can be challenging, but can potentially offer large performance gains
- Don't always count on I/O libraries or file systems to automatically provide you the best performance out of the box

Darshan is invaluable for providing understanding of application I/O behavior and informing potential tuning decisions

- https://github.com/darshan-hpc/darshan

Please reach out with questions, feedback, etc.



Thank you!

Bonus

Understanding I/O beyond the application

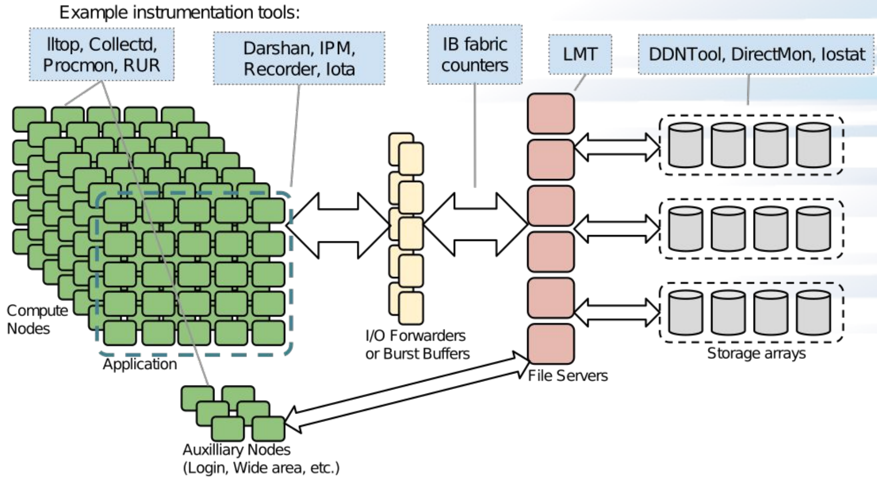
Into the wild...

Many storage resources at HPC facilities are shared between users

- Application-centric analysis can only tell us so much about HPC I/O behavior -- systems-level perspective is needed for complete picture

A more complete understanding of system I/O behavior is critical to reasoning about I/O performance

- How is my performance compared to others?
- What are the performance bottlenecks?
- How much is my I/O affected by contention?



Many existing tools can be used to help compile an accurate system-level view of I/O

Understanding I/O beyond the application

Forming a holistic view

The TOKIO (Total Knowledge of I/O) project aims to provide a framework for holistic characterization and analysis of HPC I/O workloads:

- Collect, integrate, and analyze disparate I/O data
- Define platform-independent blueprint for deploying and utilizing I/O characterization tools, data collection/storage services, and analysis methods
- Provide a trove of relevant data characterizing HPC I/O workloads

Stakeholders:

- Application scientists (productivity)
- Facility operators (efficiency)
- Researchers (optimization)

For more info: https://www.anl.gov/mcs/tokio-total-knowledge-of-io

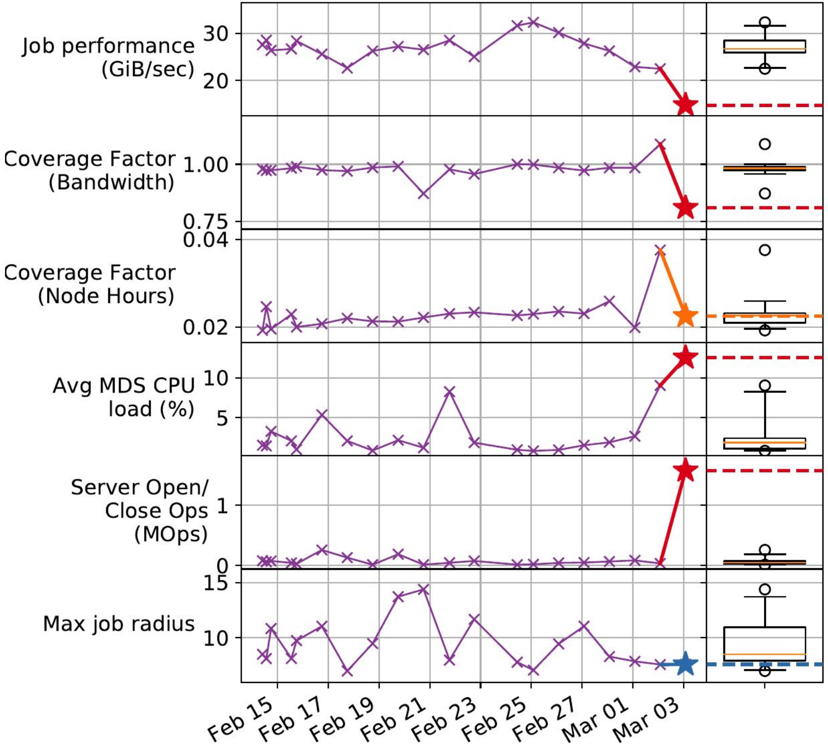
Understanding I/O beyond the application

A TOKIO example

TOKIO utility called UMAMI (Unified metrics and measurements interface) contextualizes application performance measurements with other system measurements

How does my performance compare to previous runs?

Do any metrics stand out that positively/negatively impacted my performance?



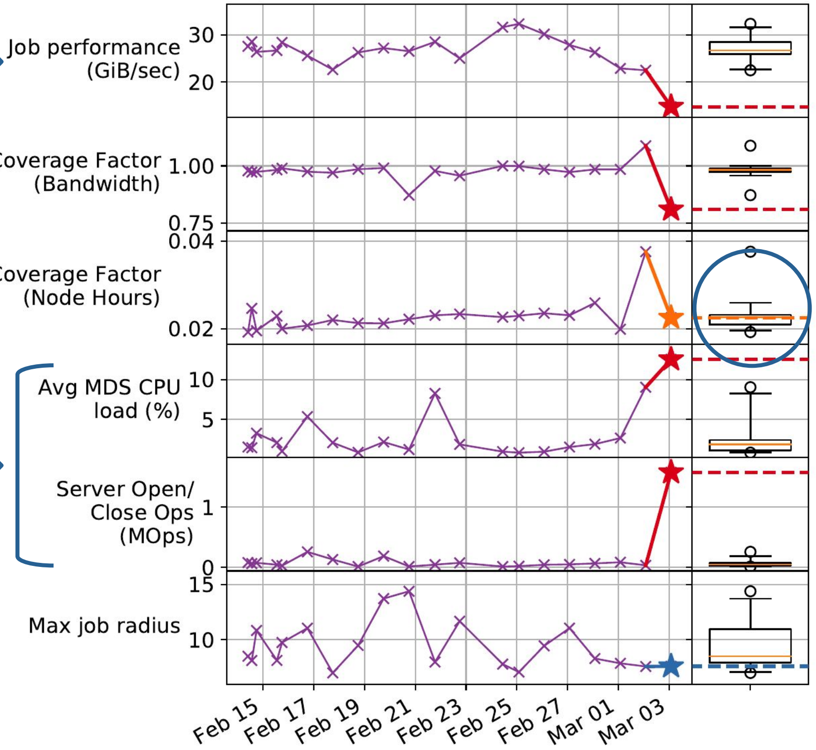
Understanding I/O beyond the application

A TOKIO example

Raw performance

Coverage factor represents contention

Metadata loads

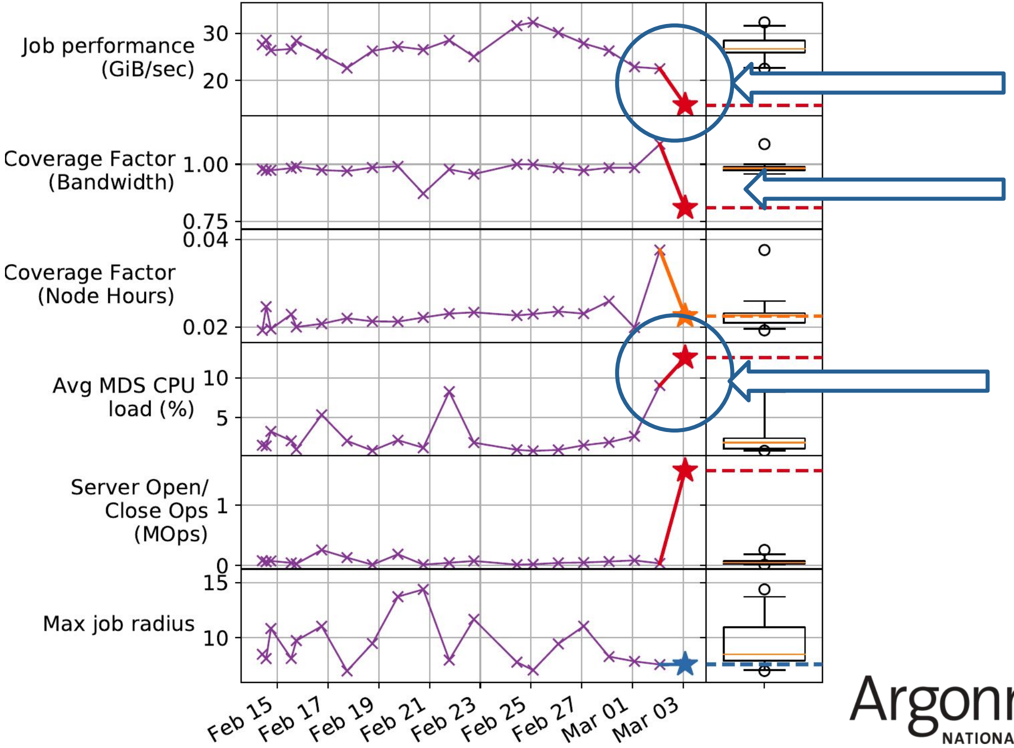


Historical measurements

Box plots to compare against historical measurements

Understanding I/O beyond the application

A TOKIO example



Low performance relative to recent runs

Low coverage factor, meaning other jobs were performing I/O while we were

High metadata server load also likely impacting performance